International Journal of Chemical Kinetics 2015 vol.47 N6, pages 389-394

New approach to determine the activation and reaction volumes of low polar molecular processes

Kornilov D., Kiselev V.
Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

Abstract

© 2015 Wiley Periodicals, Inc. For low polar molecular processes, we found the reliable relationship between the logarithm changes of the rate or equilibrium constants in the pressure range 1-1000 bar, [Ln(KP = 1000/KP = 1)/1000], and tangent modulus at P = 1 bar, ∂Ln(KP)/∂P: ∂Ln(KP)/∂P = 1.15·[Ln(KP = 1000/KP = 1)/1000], R = 0.995, which allows to predict the value of activation and reaction volume at ambient pressure. Therefore, it is sufficient to determine the values of the rate or equilibrium constants only at ambient pressures and at 1000 bar for the reliable estimation of the values of activation or reaction volume.

http://dx.doi.org/10.1002/kin.20916